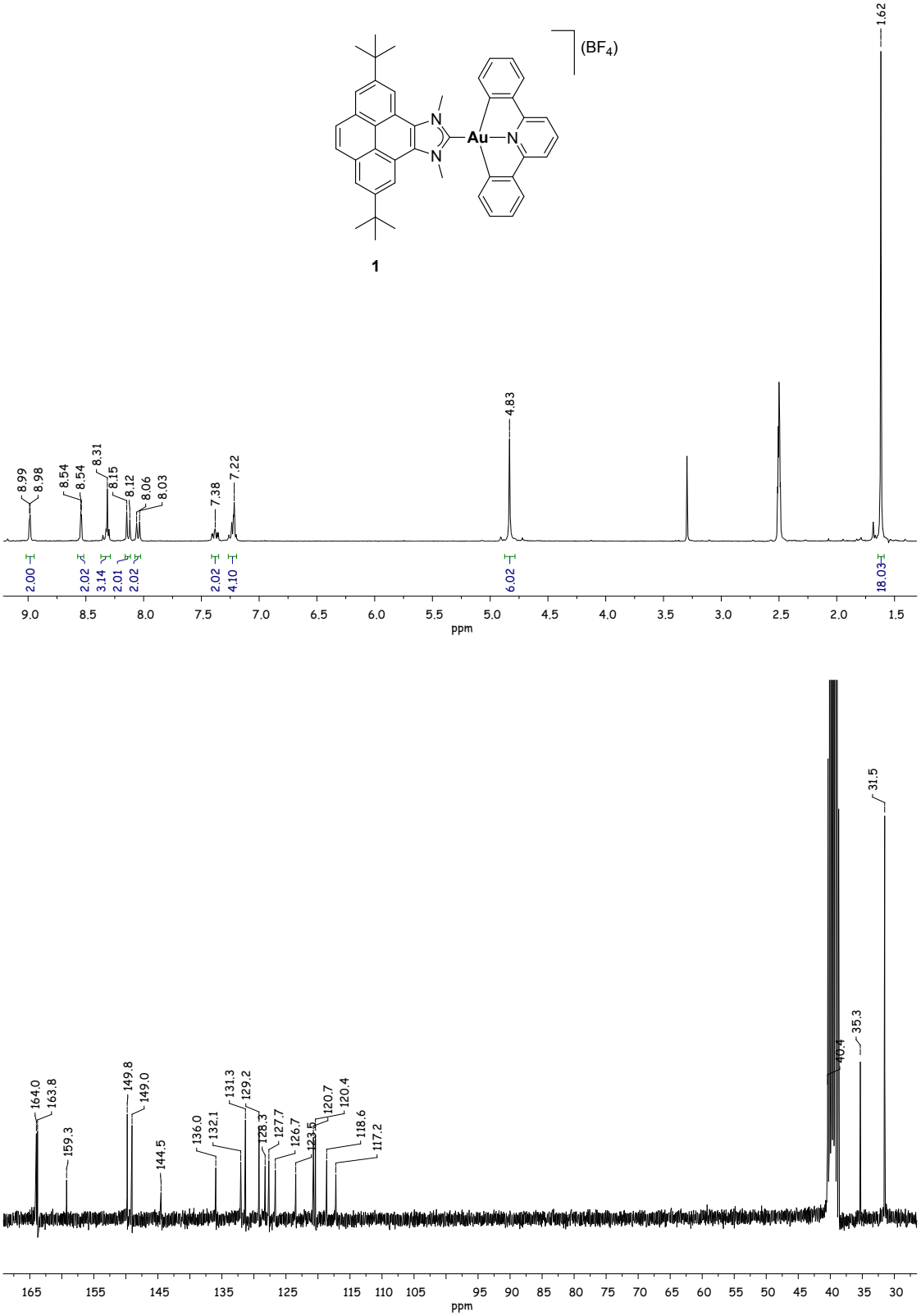
Supplementary Information for:

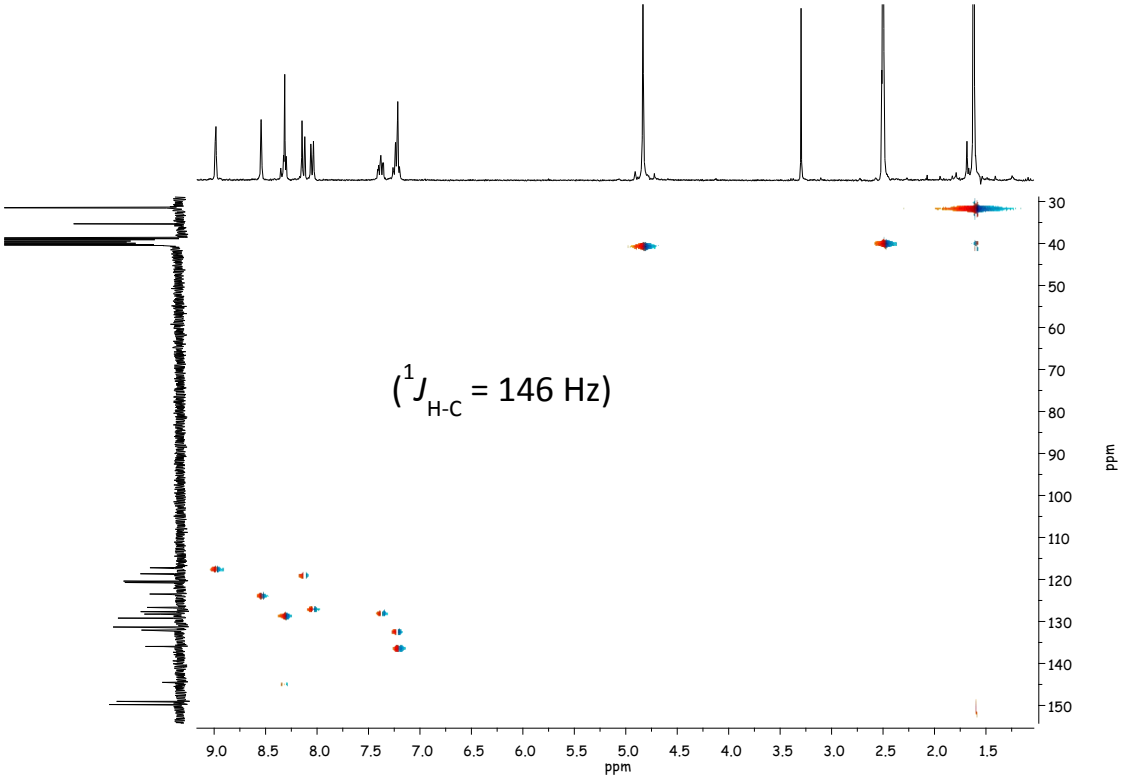
Pincer-CNC Au(III) and Pt(II) Complexes Supported by Pyrene-Based N-Heterocyclic Carbenes: Synthesis and Photophysical Properties

by Sergio Gonell, Macarena Poyatos and Eduardo Peris

1. Spectroscopic data

1.1 ^{1}H, ^{13}C and HSQC NMR spectra of **1**

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8.5
8.0
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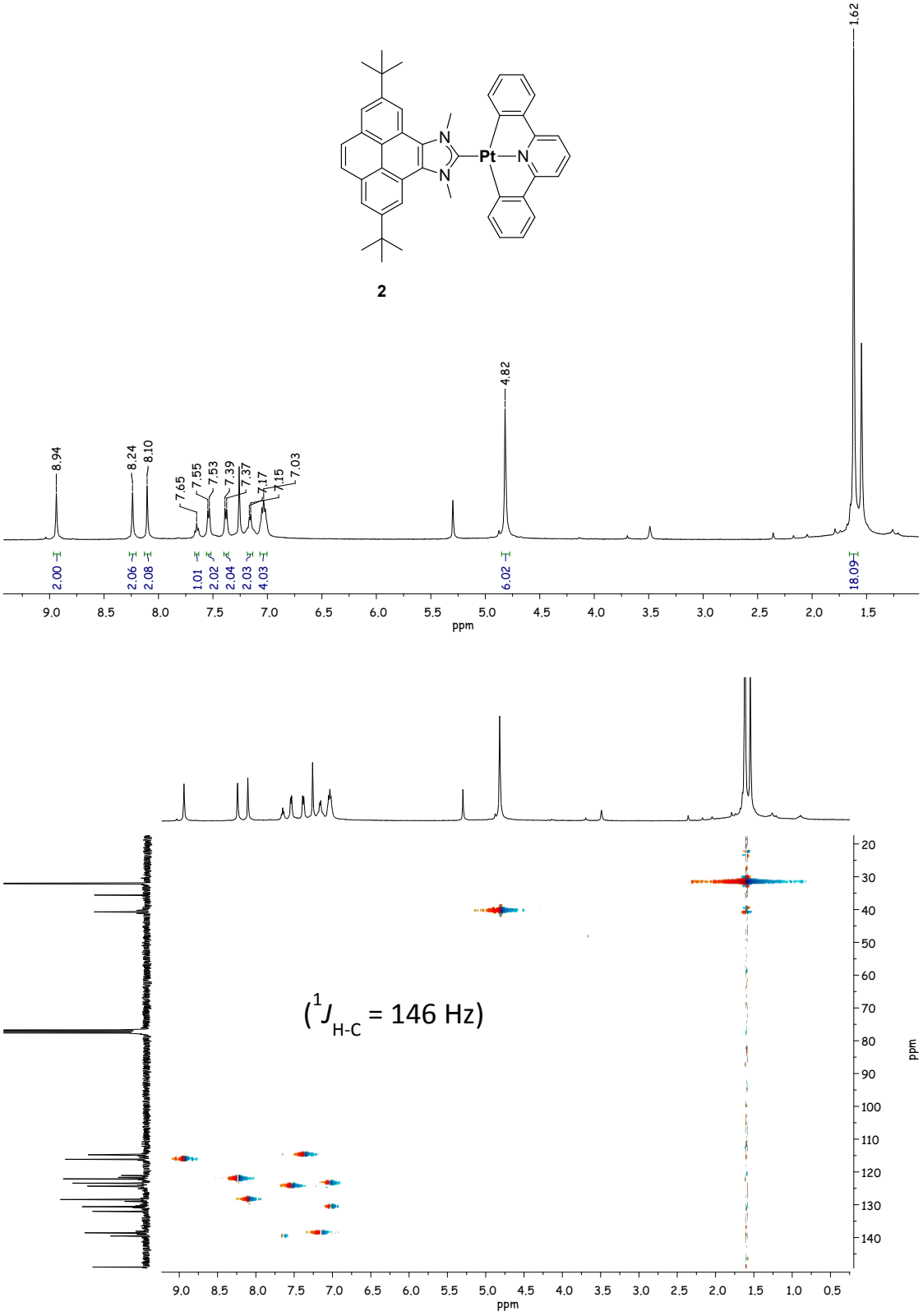
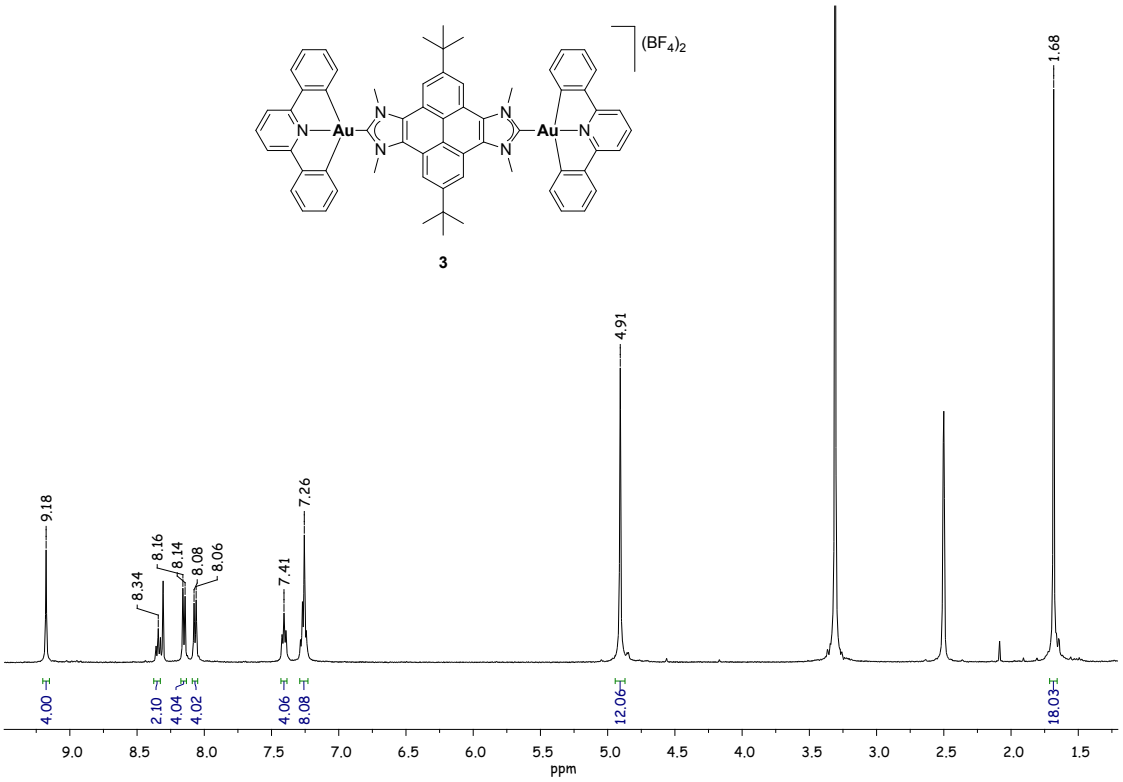
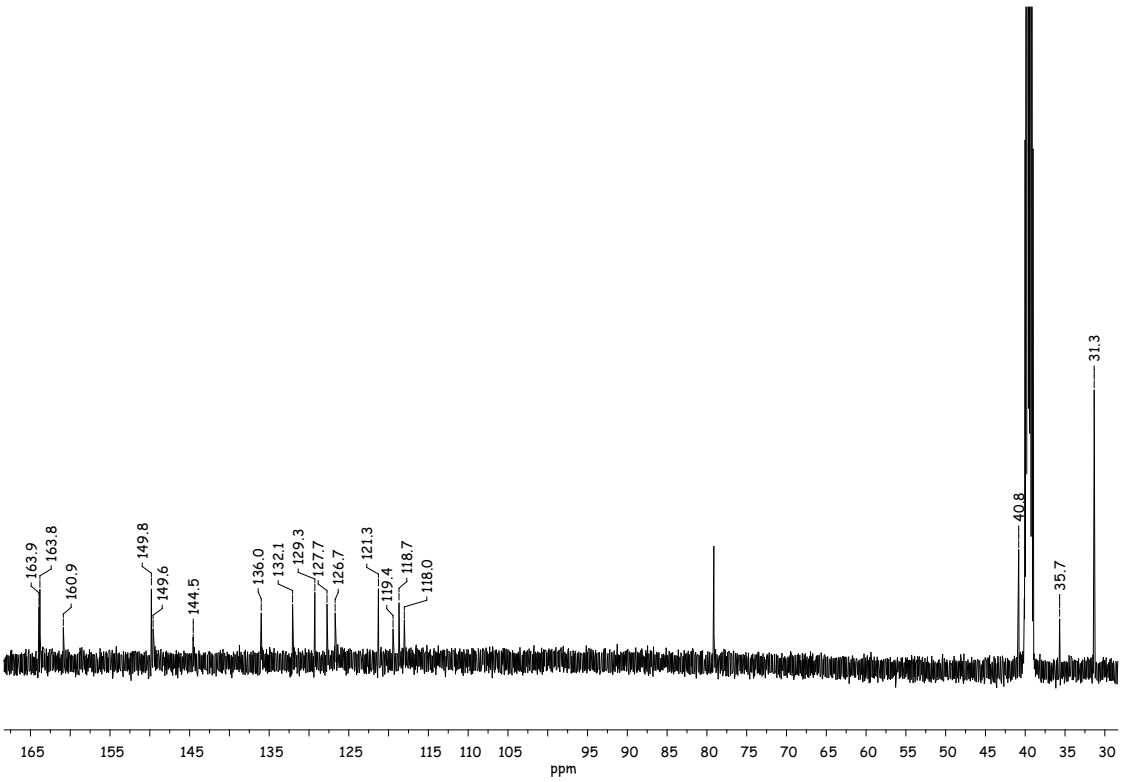
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm

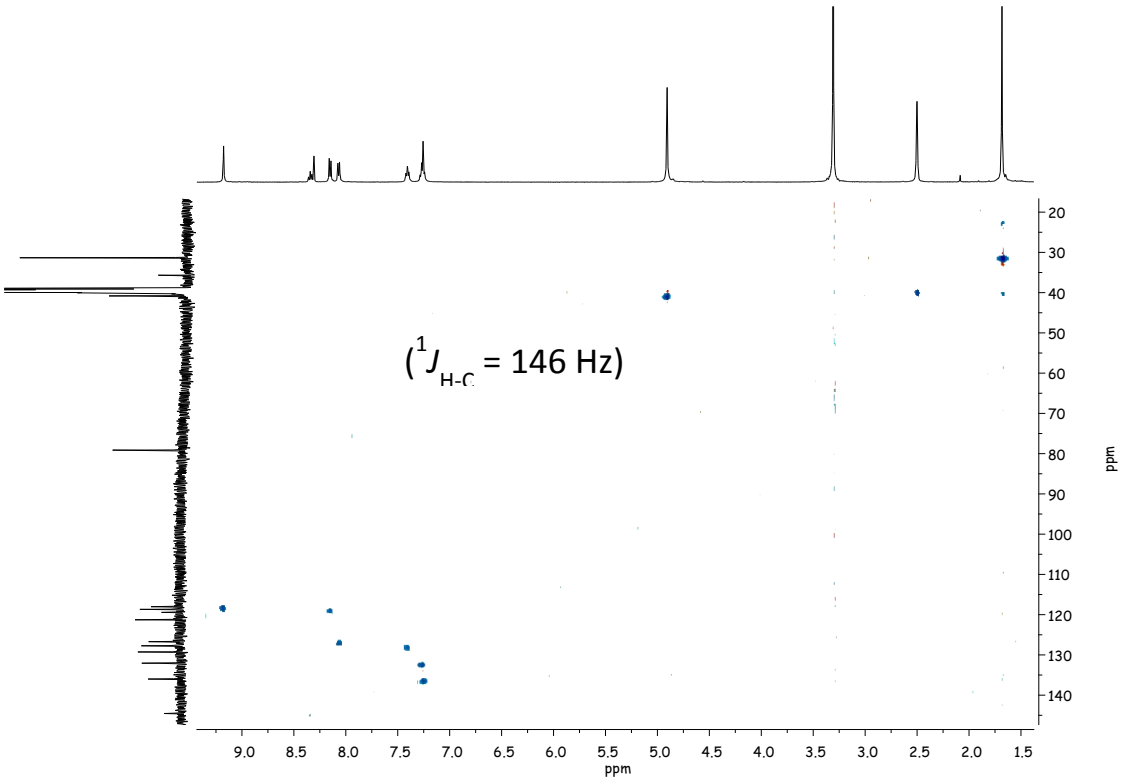
1.2 ^{1}H, ^{13}C and HSQC NMR spectra of **2**



1.3 ^{1}H, ^{13}C and HSQC NMR spectra of **3**



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4.0
3.5
3.0
2.5
2.0
1.5
ppm
20
30
40
50
60
70
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90
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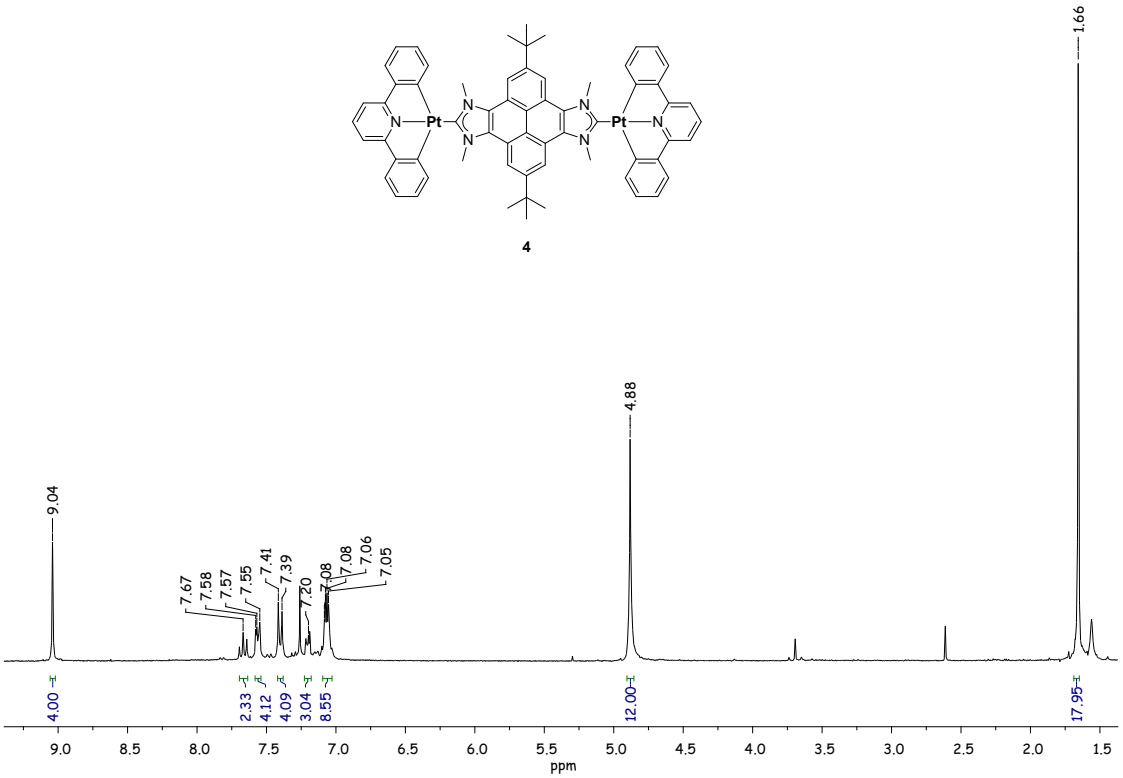
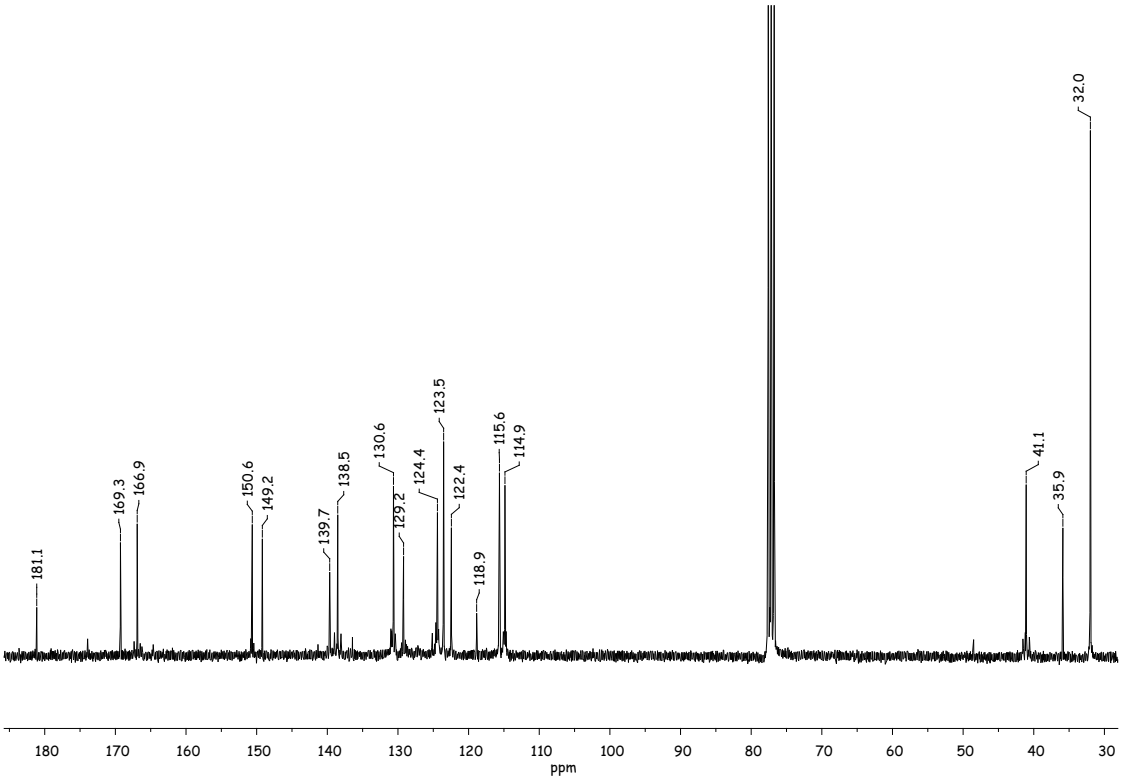
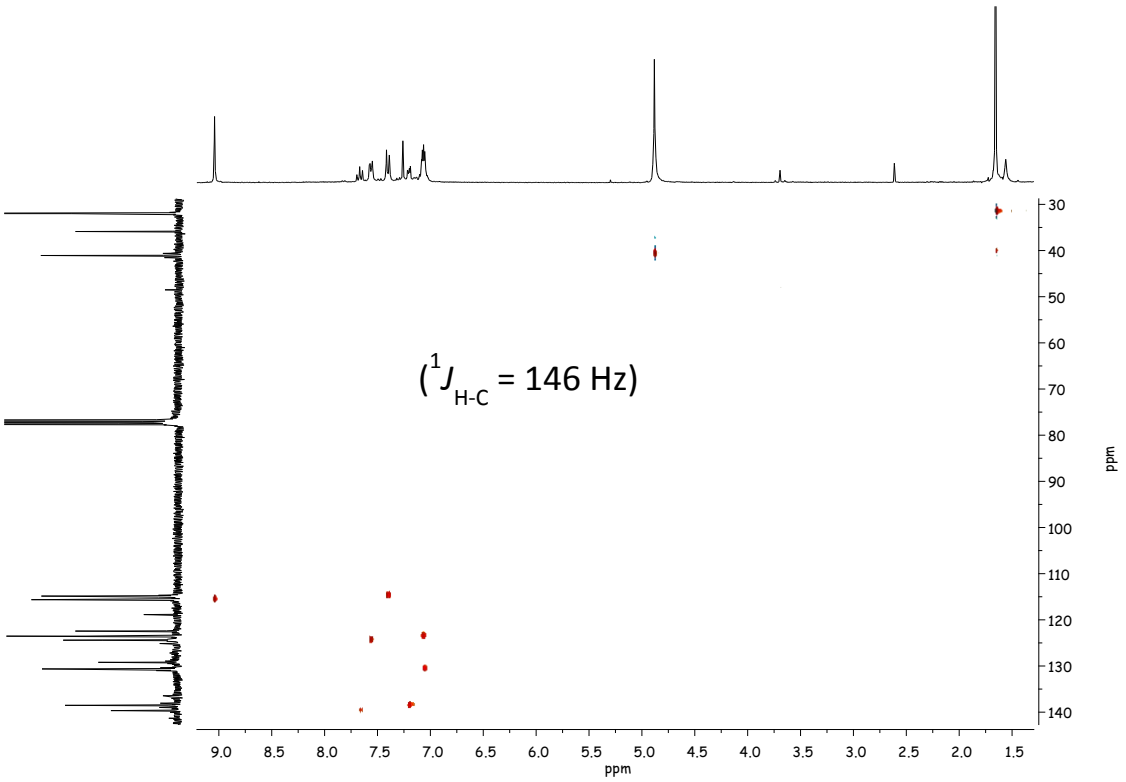
ppm

1.4 ^{1}H, ^{13}C and HSQC NMR spectra of **4**

4



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7.0
6.5
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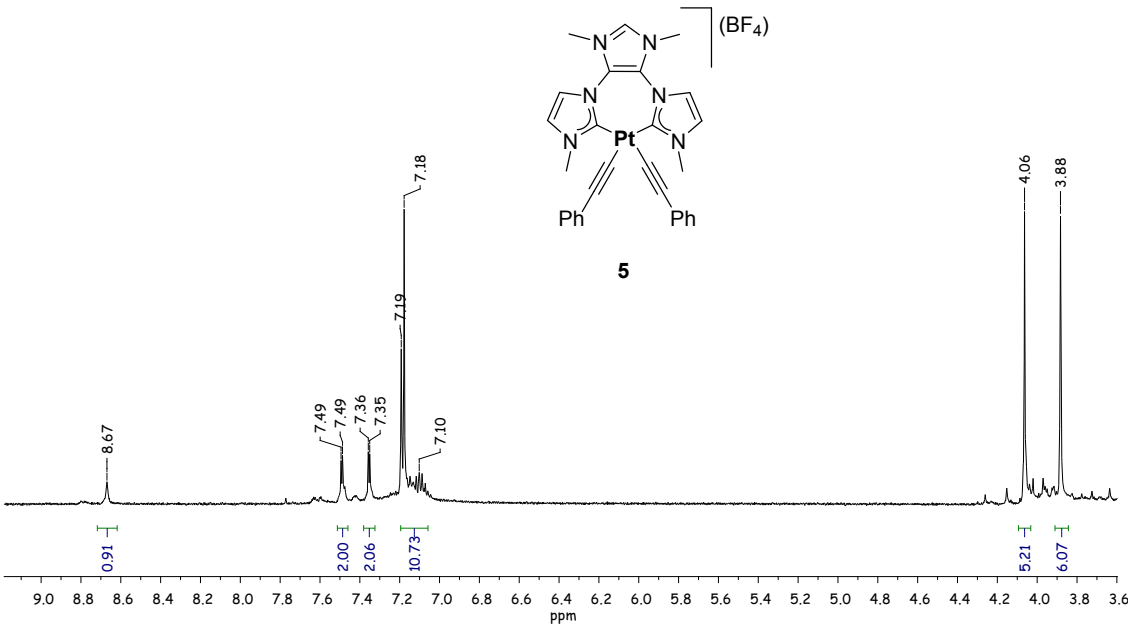
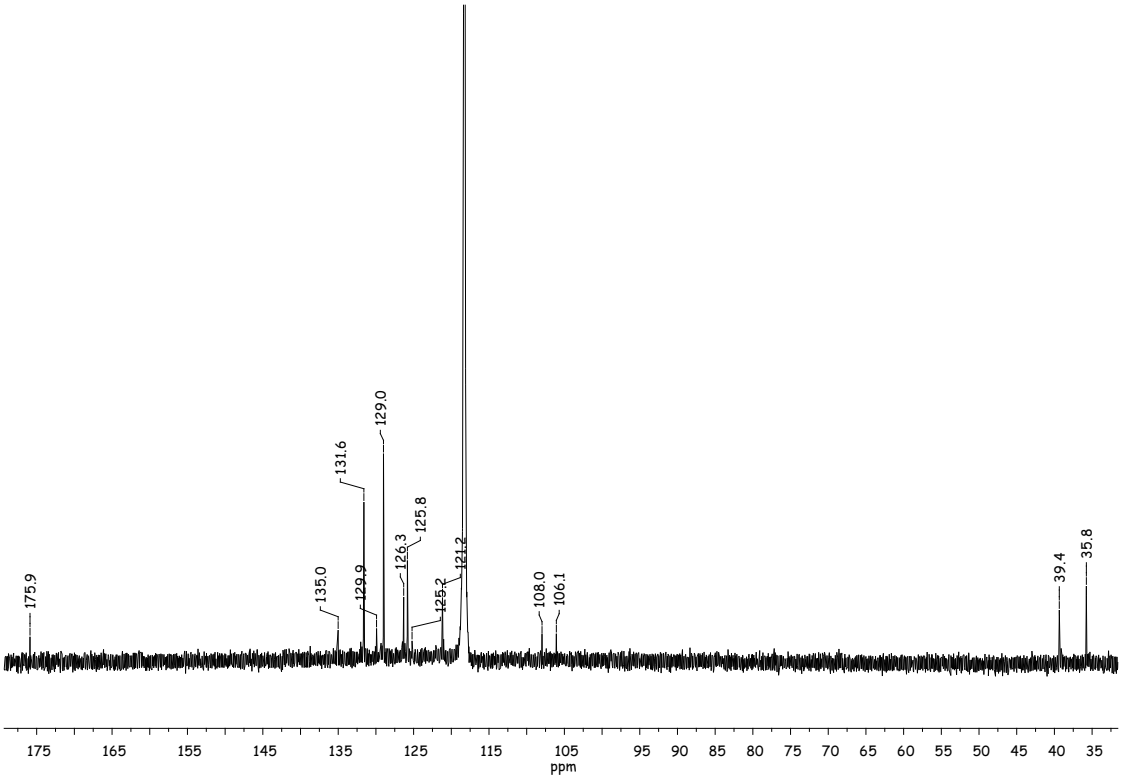
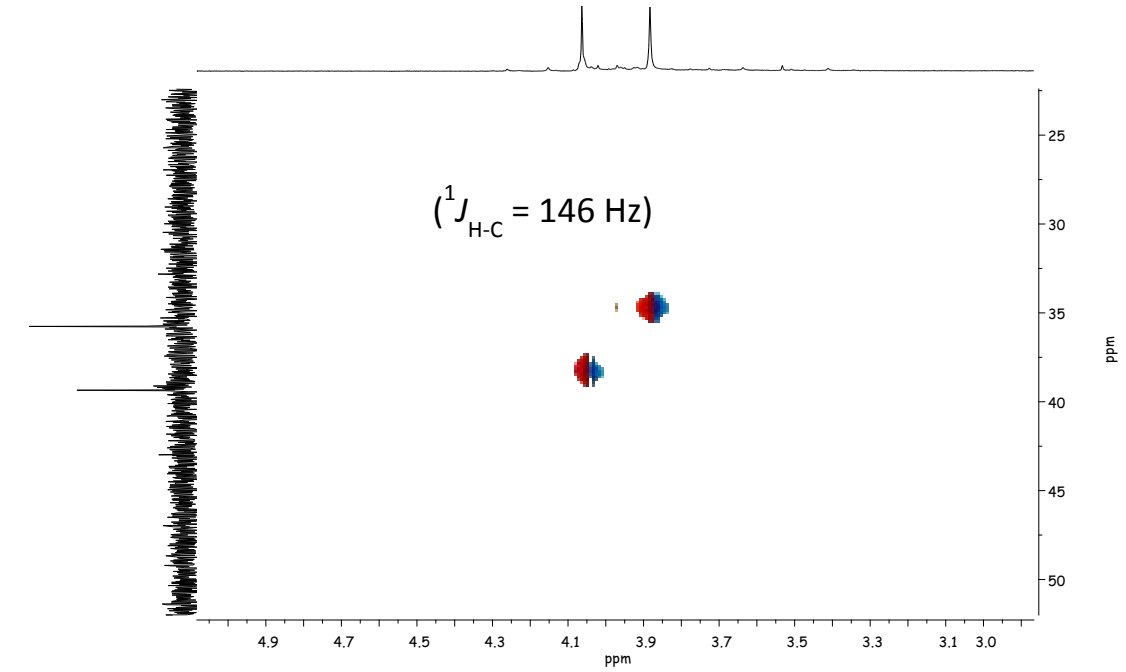
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
30
40
50
60
70
80
90
100
110
120
130
140
ppm

1.5 ^{1}H, ^{13}C and HSQC NMR spectra of **5**



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25
30
35
40
45
50
ppm
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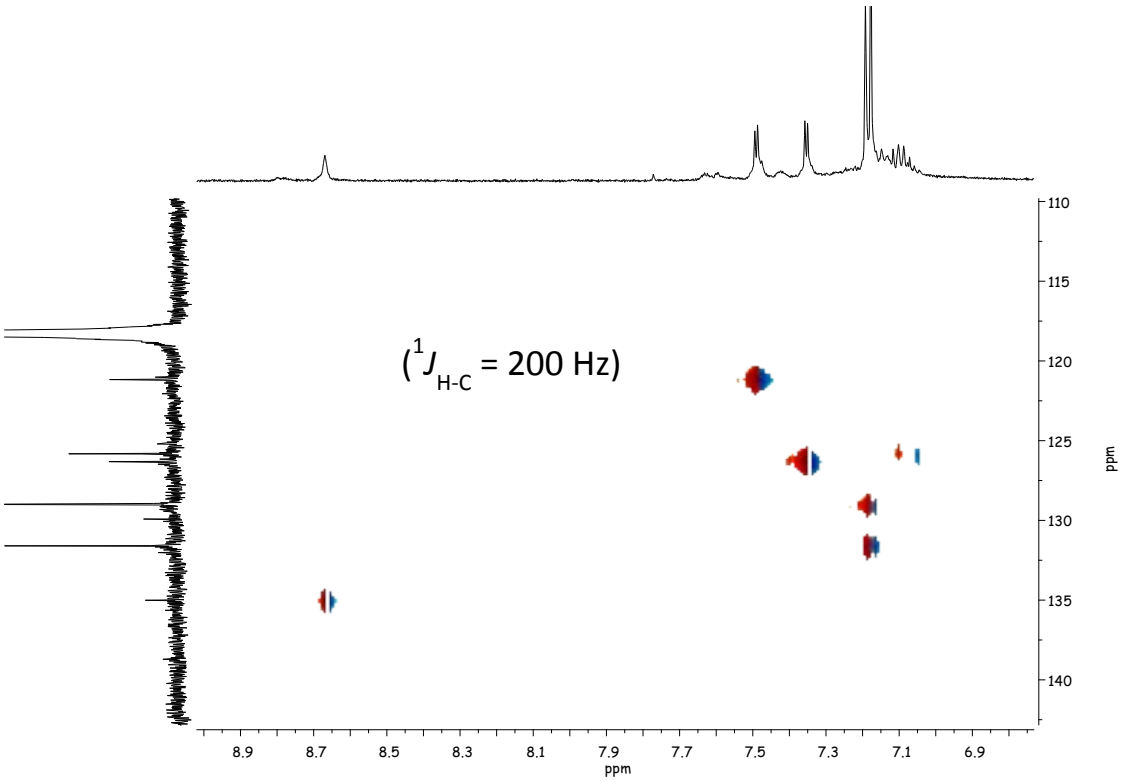
4.5
4.3
4.1
3.9
3.7
3.5
3.3
3.1
3.0
ppm


($^1J_{H-C}$ = 200 Hz)
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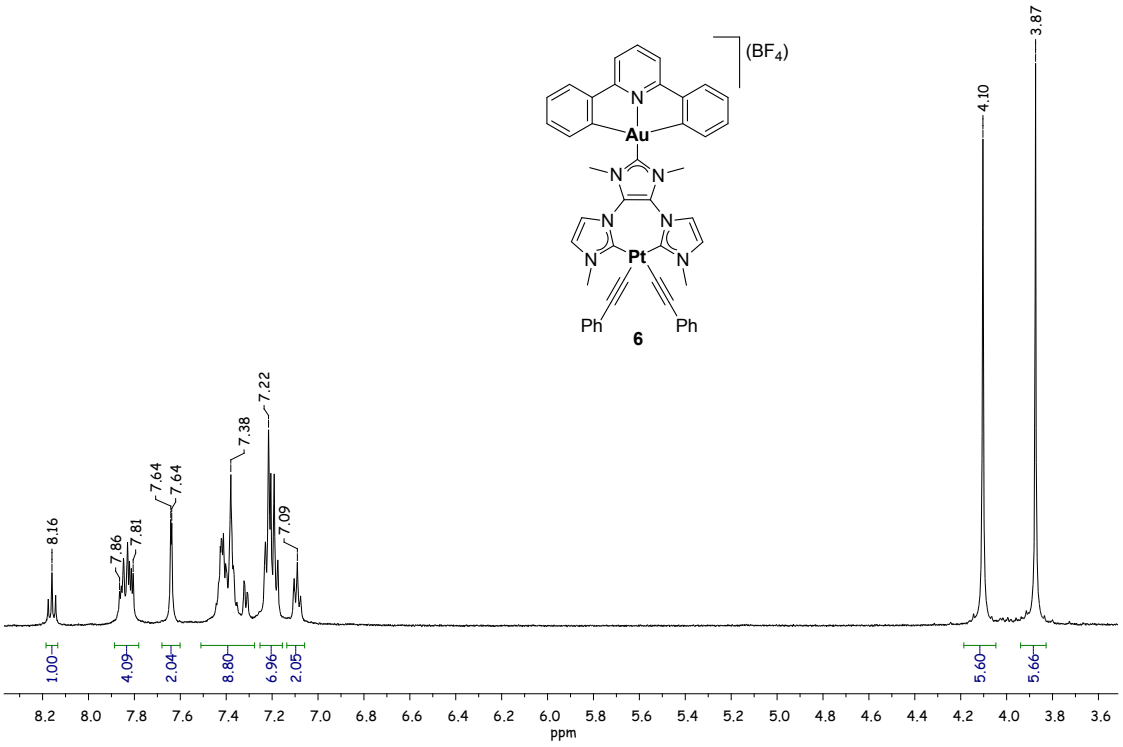
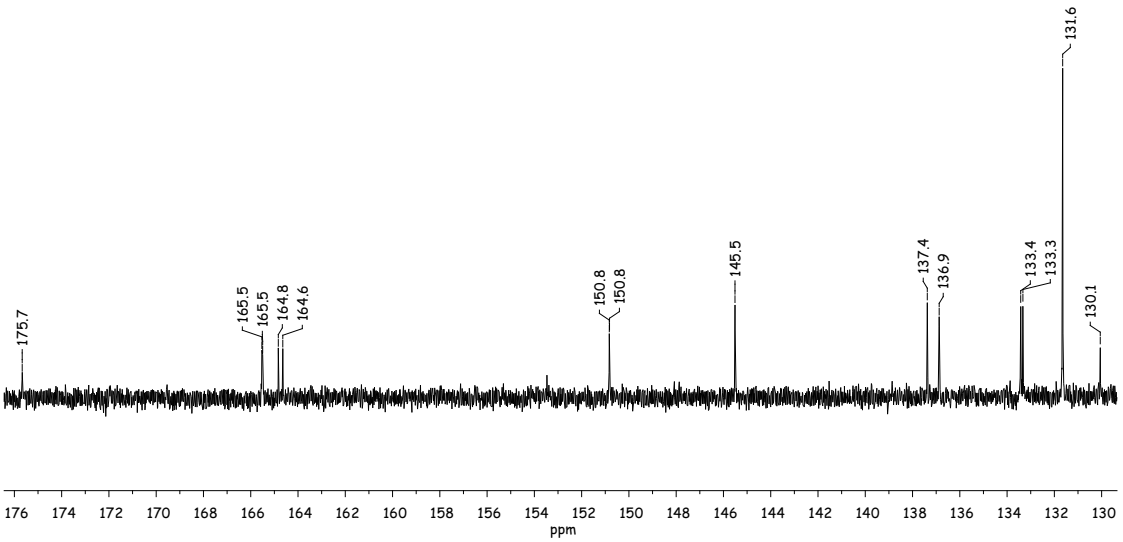
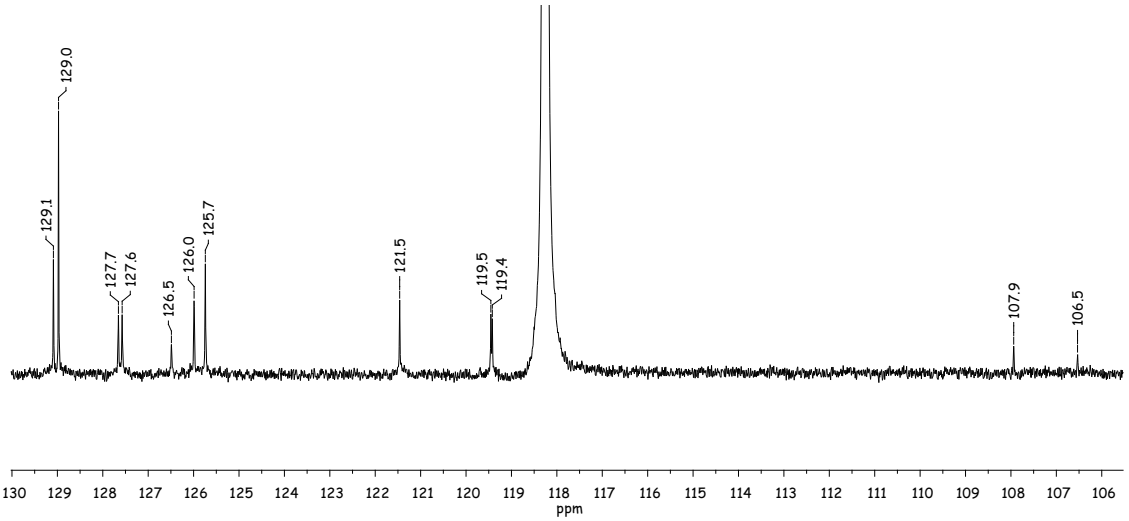
115
120
125
130
135
140
ppm
8.9
8.7
8.5
8.3
8.1
7.9
7.7
7.5
7.3
7.1
6.9
ppm

1.6 ^{1}H, ^{13}C and HSQC NMR spectra of **6**



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127.6
126.5
126.0
125.7
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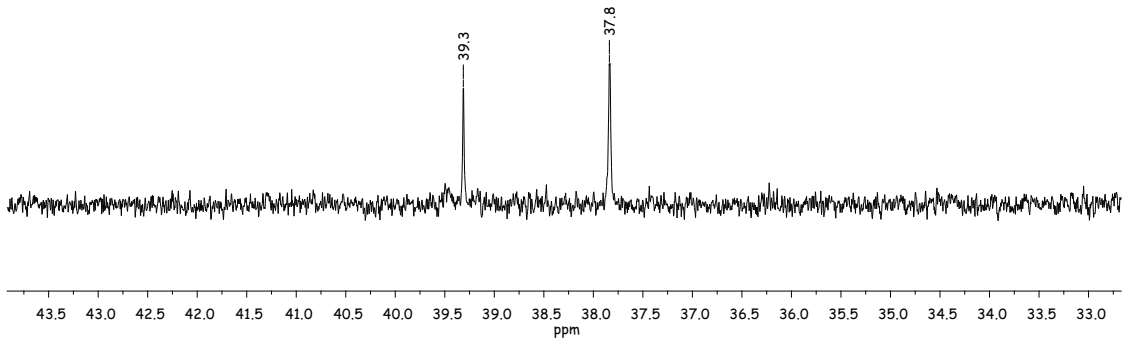
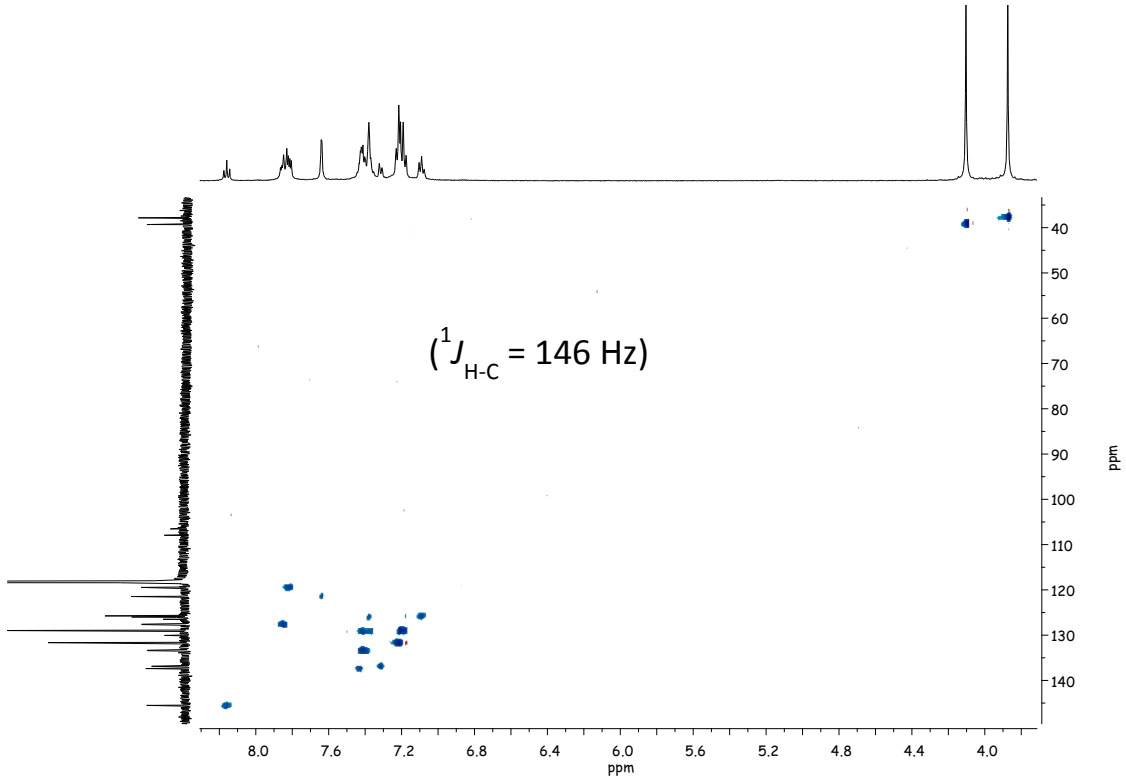
119.5
119.4
107.9
106.5
ppm


39.3
37.8
ppm


($^{1}J_{H-C}$ = 146 Hz)
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ppm

2. UV-Vis and emission spectra

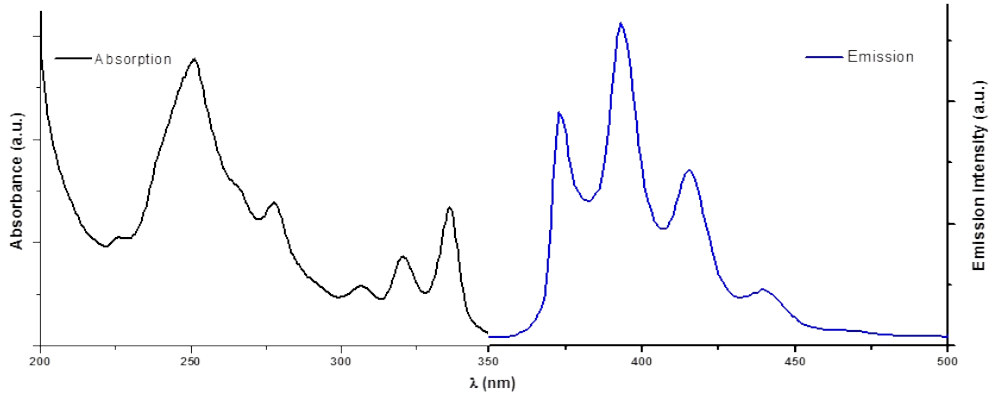

Figure S1. UV-Vis and emission spectra of mono-imidazolium salt **A**, recorded in MeCN

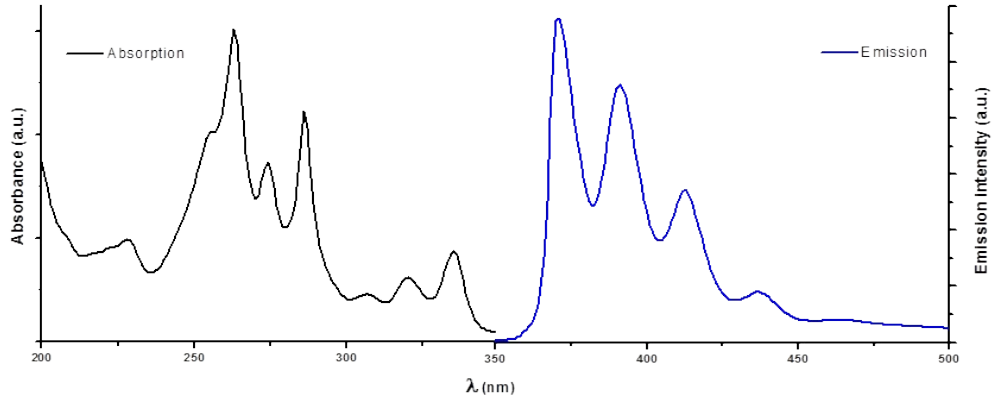

Figure S2. UV-Vis and emission spectra of mono-imidazolium salt **B**, recorded in MeCN

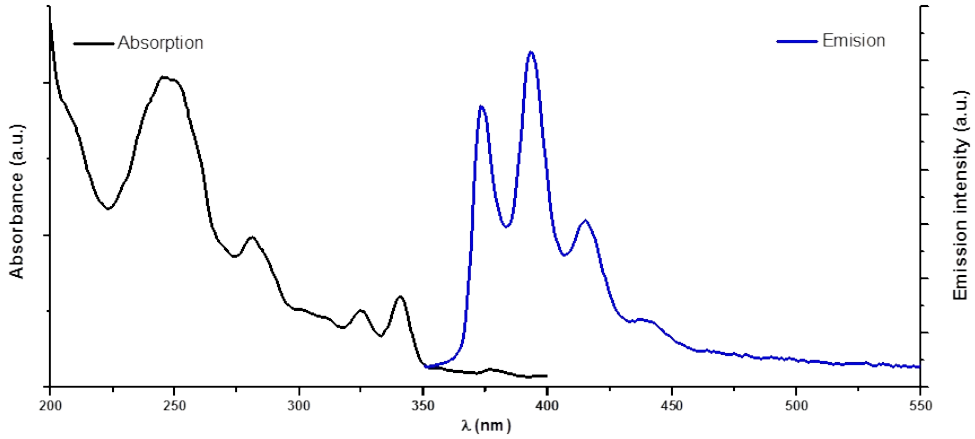

Figure S3. UV-Vis and emission spectra of complex **1** recorded in MeCN

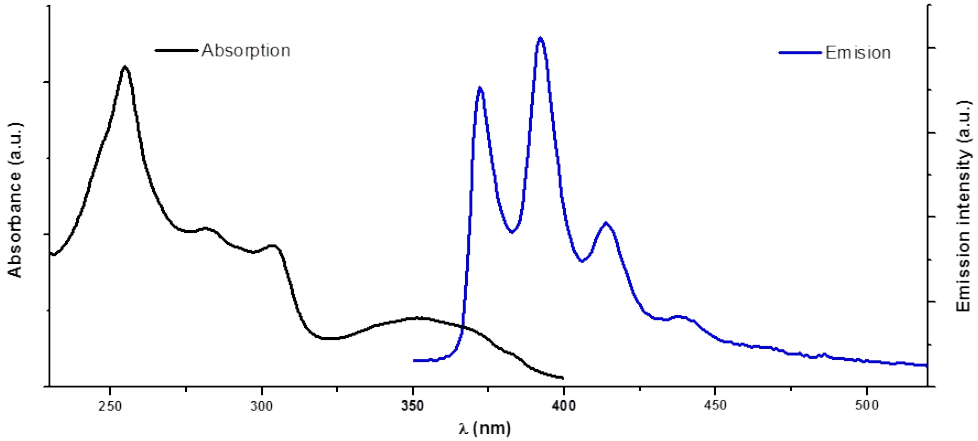

Figure S4. UV-Vis spectrum (recorded in CH_2Cl_2) and emission spectrum (recorded in MeCN) of complex **2**

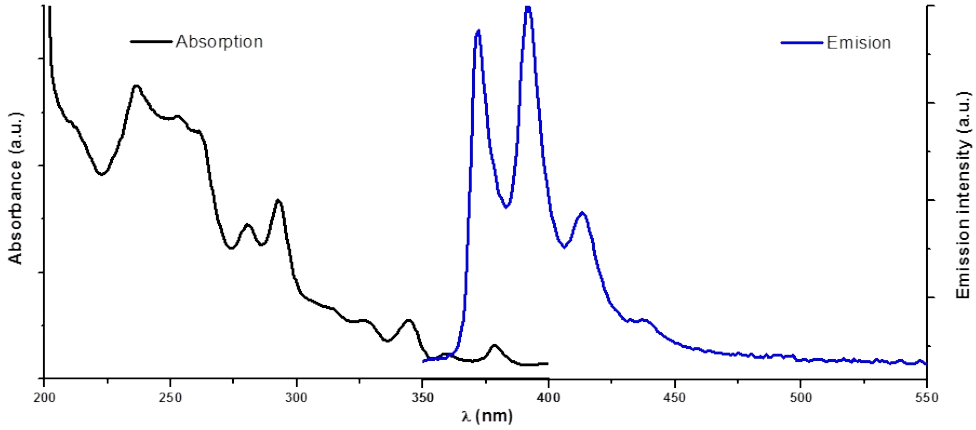

Figure S5. UV-Vis and emission spectra of complex **3** recorded in MeCN

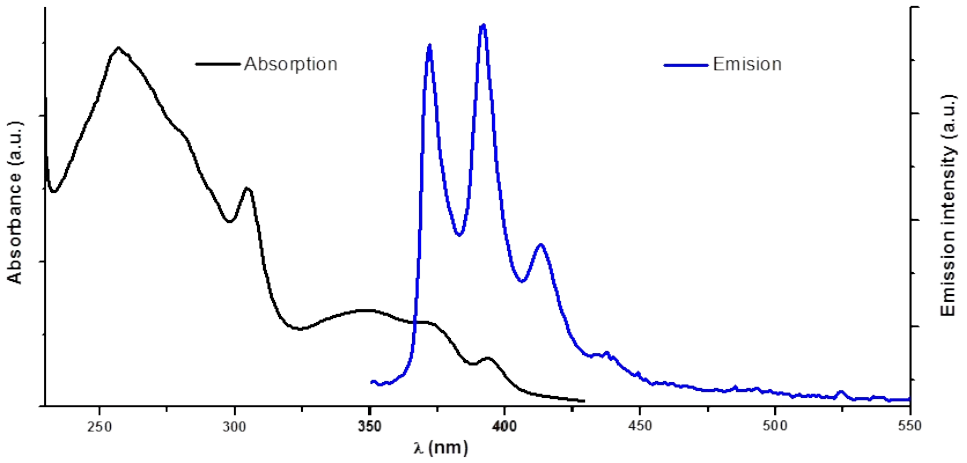

Figure S6. UV-Vis spectrum (recorded in CH_2Cl_2) and emission spectrum (recorded in MeCN) of complex **4**

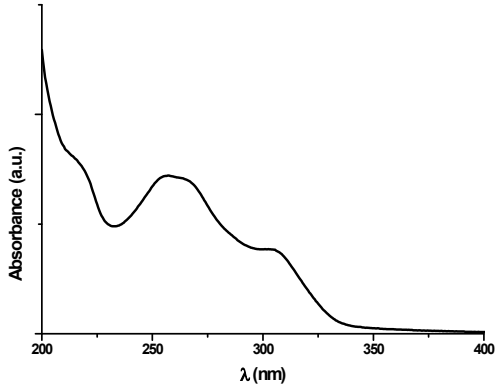

Figure S7. UV-Vis spectrum of complex **5** recorded in MeCN

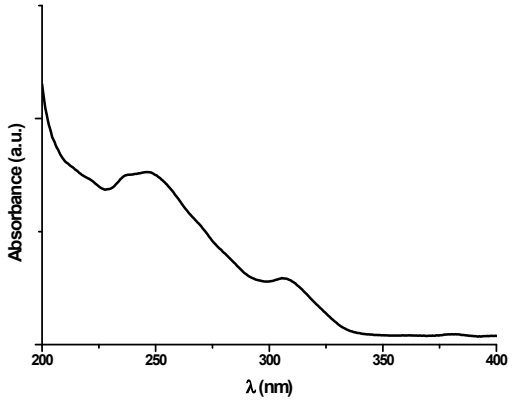

Figure S8. UV-Vis spectrum of complex **6** recorded in MeCN

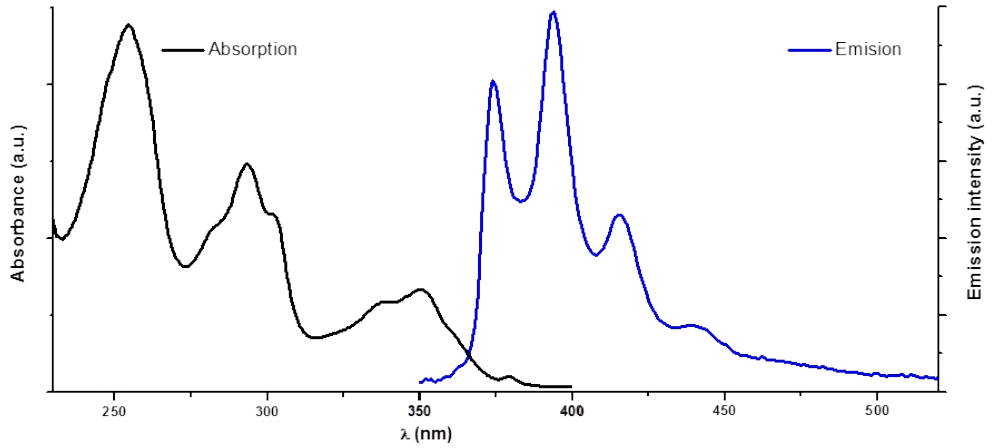

Figure S9. UV-Vis spectrum (recorded in CH_2Cl_2) and emission spectrum (recorded in MeCN) of complex **7**

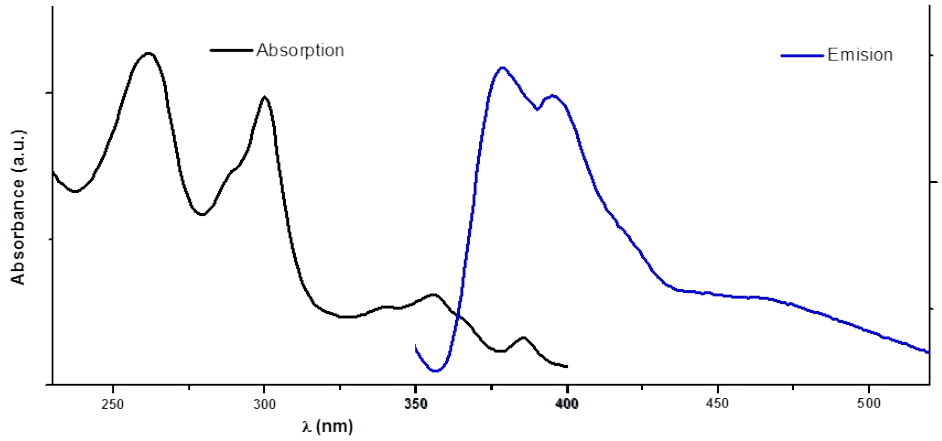

Figure S10. UV-Vis spectrum (recorded in CH_2Cl_2) and emission spectrum (recorded in MeCN) of complex **8**

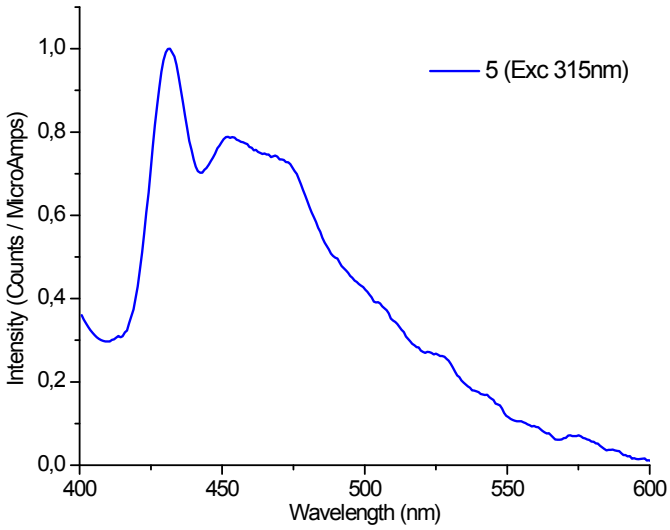

Figure S11. Normalized emission of complex **5** at 5 wt% in PMMA

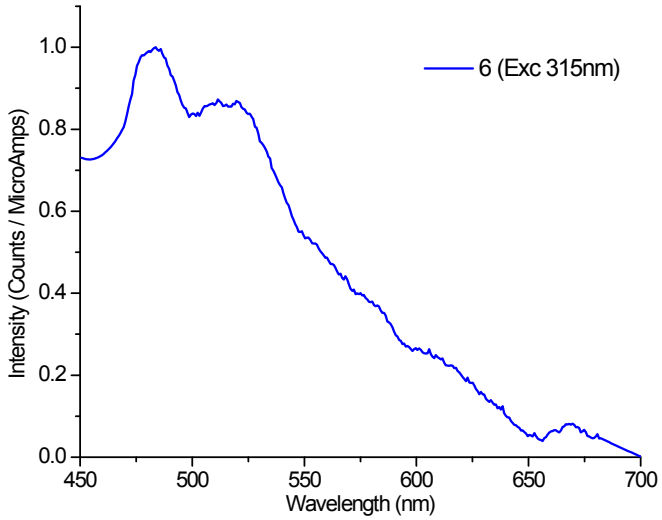

Figure S12. Normalized emission of complex **6** at 10 wt% in PMMA

3. Cyclic voltammetry studies

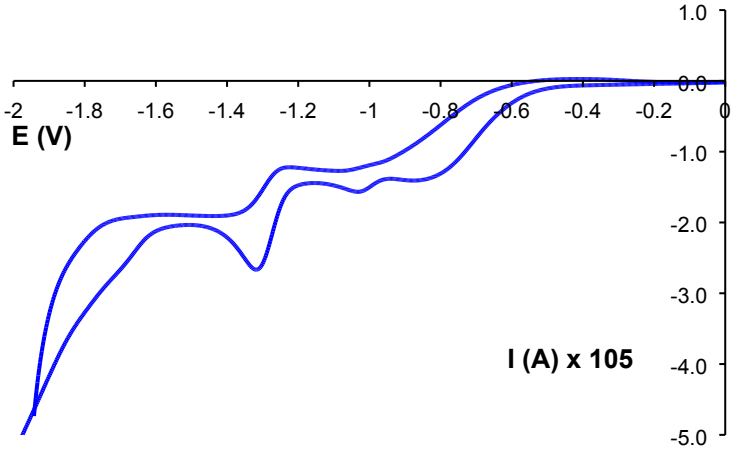

Figure S13. Cyclic voltammogram of complex **1**

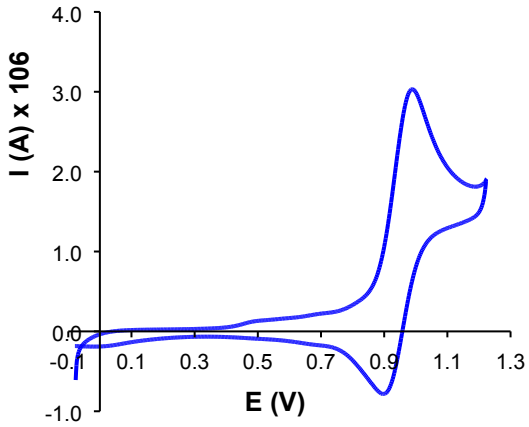

Figure S14. Cyclic voltammetry of complex **2**

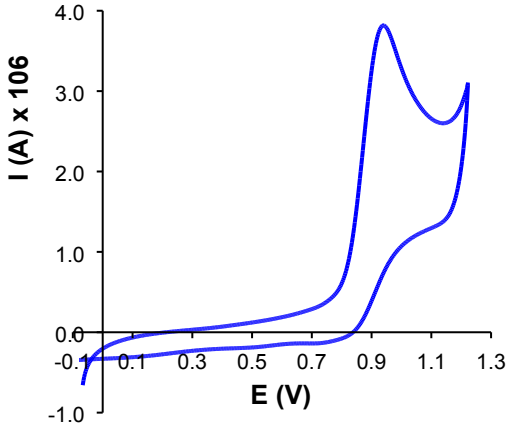

Figure S15. Cyclic voltammetry of complex **4**

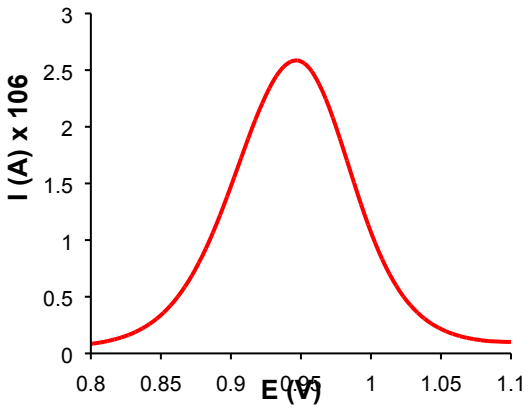

Figure S16. Relevant DPV section of complex **2**

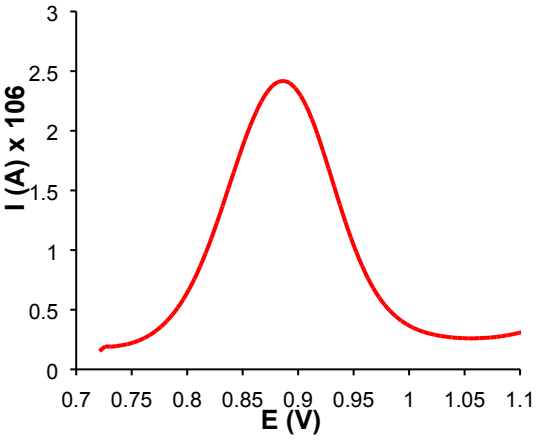

Figure S17. Relevant DPV section of complex **4**

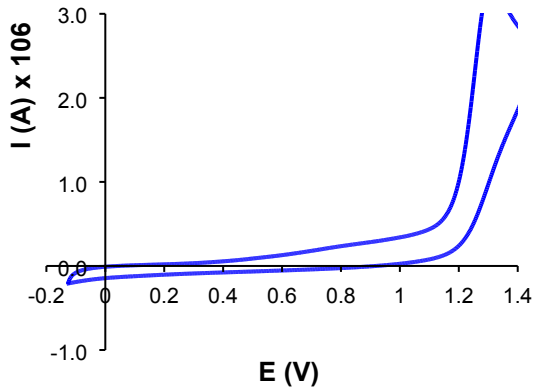

Figure S18. Cyclic voltammetry of complex **5**

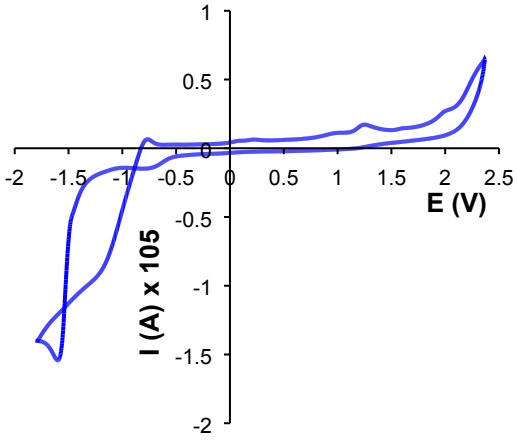

Figure S19. Cyclic voltammetry of complex **6**

4. X-Ray crystallography

X-Ray diffraction studies for 4. Crystals suitable for X-ray study of compound **4** were obtained by slow diffusion of hexane into a concentrated solution of the complex in chloroform. Diffraction data was collected on an Agilent SuperNova diffractometer equipped with an Atlas CCD detector. Single crystals were mounted on a MicroMount® polymer tip (MiteGen) in a random orientation. The structure was solved by direct methods in SHELXS-97 and refined by the full-matrix method based on F^2 with the program SHELXL-97 using the OLEX software package.[1] Key details of the crystal and structure refinement data are summarized in Supplementary Table S1. Further crystallographic details may be found in the CIF which was deposited at the Cambridge Crystallographic Data Centre, Cambridge, UK. The reference number for **4** was assigned as 1446681.

Supplementary Table S1. Summary of crystal data, data collection, and structure refinement details.

Empirical formula	$C_{66}H_{60}Cl_4N_6Pt_2$
Formula weight	1469.18
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	18.3864(6)
b/Å	10.9440(3)
c/Å	15.1682(5)
α/°	90.00
β/°	111.100(4)
γ/°	90.00
Volume/Å^3	2847.51(15)
Z	2
ρ_{calc}g/cm^3	1.714
μ/mm^{-1}	5.143
F(000)	1444.0
Crystal size/mm^3	0.2267 × 0.2096 × 0.1698
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.72 to 52
Index ranges	$-22 \le h \le 22$, $-12 \le k \le 13$, $-18 \le l \le 18$
Reflections collected	28273
Independent reflections	5587 [R_{int} = 0.0413, R_{sigma} = 0.0271]
Data/restraints/parameters	5587/0/357
Goodness-of-fit on F^2	1.113
Final R indexes [I>=2σ (I)]	R_1 = 0.0346, wR_2 = 0.0816
Final R indexes [all data]	R_1 = 0.0378, wR_2 = 0.0837
Largest diff. peak/hole / e Å^{-3}	1.48/-1.22

5. References

(1) (a) Sheldrick, G. M. *Acta Crystallogr. Sect. A* **2008**, *64*, 112-122; (b) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Crystallogr.* **2009**, *42*, 339-341.